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201-16554C

I U C L I D

Data Set

Existing Chemical : ID: 68515-41-3
CAS No. : 68515-41-3
EINECS Name : 1,2-Benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
EC No. : 271-083-0
IUPAC Name : 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters

Producer related part
Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 04.10.2001

Substance related part
Company : ExxonMobil Biomedical Sciences Inc.
Creation date : 04.10.2001

Status :
Memo : ACC Phthalate Ester Panel HPV Testing Group

Printing date : 07.12.2006
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Number of pages : 32

Chapter (profile) : Chapter: 1, 2, 3, 4, 5, 6, 7, 8, 10
Reliability (profile) : Reliability: without reliability, 1, 2, 3, 4
Flags (profile) : Flags: without flag, confidential, non confidential, WGK (DE), TA-Luft (DE),
Material Safety Dataset, Risk Assessment, Directive 67/548/EEC, SIDS

1.0.1 APPLICANT AND COMPANY INFORMATION

1.0.2 LOCATION OF PRODUCTION SITE, IMPORTER OR FORMULATOR

1.0.3 IDENTITY OF RECIPIENTS

1.0.4 DETAILS ON CATEGORY/TEMPLATE

Comment : This chemical is not a member of the High Molecular Weight Phthalate Esters subcategory but its data are being used to support a hazard assessment of the subcategory. The subcategory includes eleven CAS numbers (See Fretext Remark)

Remark : This chemical is not a member of the High Molecular Weight Phthalate Esters subcategory but its data are being used to support a hazard assessment of the subcategory. The subcategory includes the following eleven CAS numbers:

68648-93-1	1,2-benzenedicarboxylic acid, mixed decyl and hexyl and octyl diesters (610P)
117-84-0	1,2-benzenedicarboxylic acid, dioctyl ester (DOP)
16883-83-3	1,2-Benzenedicarboxylic acid, benzyl 3-hydroxy-1-isopropyl-2,2-dimethylpropyl ester isobutyrate (B84P)
68515-40-2	1,2-benzenedicarboxylic acid, benzyl C7-9 branched and linear alkyl (B79P)
68515-45-7	1,2-benzenedicarboxylic acid, dinonyl ester, branched and linear (DNP)
68515-43-5	1,2-Benzenedicarboxylic acid, di-C9-11-branched and linear alkyl esters (911P)
84-77-5	1,2-benzenedicarboxylic acid, didecyl ester (DDP)
3648-20-2	1,2-benzenedicarboxylic acid, diundecyl ester (DUP)
85507-79-5	1,2-benzenedicarboxylic acid, di (C11) ester, branched and linear (DinUP)
111381-91-0	1,2-benzenedicarboxylic acid (C9, C11) ester, branched and linear (Din911P)
68515-47-9	1,2-benzenedicarboxylic acid, di-C11-14-branched alkyl esters, C13 rich (DTDP)

The phthalate esters comprise a family of chemicals synthesized by esterifying phthalic anhydride with various alcohols in the presence of an acid catalyst. Phthalate esters are all 1,2-benzenedicarboxylic acids with side chain ester groups ranging from C1 to approximately C13. The structural characteristics of the ester side chains affect both the physical/chemical and biological properties of phthalate esters.

Phthalate esters are generally clear to yellow, oily liquids with high boiling ranges (>250°C) and low vapor pressures; properties which contribute to their high physical stability. They are readily soluble in most organic solvents and miscible with alcohol, ether and most oils. The aqueous solubility of phthalate esters is inversely related to their molecular weights. Lower molecular weight phthalates exhibit slight to moderate water solubility, whereas, higher molecular weight phthalates exhibit very low solubility.

The phthalate esters were subdivided into three subcategories based on

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their physicochemical and toxicological properties. The phthalate esters in this subcategory, High molecular weight phthalates, are produced from alcohols with straight-chain carbon backbones of >C7 or a ring structure.

Eleven of the U.S. HPV chemicals fall into this subcategory, which includes phthalates containing linear and branched diheptyl, dioctyl, dinonyl, didecyl, diundecyl, and ditridecyl alkyl groups. This subcategory also includes phthalates that can contain a benzyl group. Data for this subcategory were supplemented with published information on other phthalate esters currently being assessed under the OECD SIDS program, including diisononyl (DINP) and diisodecyl (DIDP) phthalate.

High molecular weight phthalates are used nearly exclusively as plasticizers of PVC. They are very insoluble in water, and have a very low vapor pressure. The extant database demonstrates that these substances have few biological effects.

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1.1.0 SUBSTANCE IDENTIFICATION

1.1.1 GENERAL SUBSTANCE INFORMATION

1.1.2 SPECTRA

1.2 SYNONYMS AND TRADENAMES

1.3 IMPURITIES

1.4 ADDITIVES

1.5 TOTAL QUANTITY

1.6.1 LABELLING

1.6.2 CLASSIFICATION

1.6.3 PACKAGING

1.7 USE PATTERN

Type of use : industrial
Category : Polymers industry
Remark : High molecular weight phthalates are used nearly exclusively as

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plasticizers of PVC.

1.7.1 DETAILED USE PATTERN

1.7.2 METHODS OF MANUFACTURE

1.8 REGULATORY MEASURES

1.8.1 OCCUPATIONAL EXPOSURE LIMIT VALUES

1.8.2 ACCEPTABLE RESIDUES LEVELS

1.8.3 WATER POLLUTION

1.8.4 MAJOR ACCIDENT HAZARDS

1.8.5 AIR POLLUTION

1.8.6 LISTINGS E.G. CHEMICAL INVENTORIES

1.9.1 DEGRADATION/TRANSFORMATION PRODUCTS

1.9.2 COMPONENTS

1.10 SOURCE OF EXPOSURE

1.11 ADDITIONAL REMARKS

1.12 LAST LITERATURE SEARCH

1.13 REVIEWS

2. Physico-Chemical Data

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2.1 MELTING POINT

Value	:	= -48 - -45 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	
Year	:	
GLP	:	
Test substance	:	other TS: CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Remark	:	Manufacturer's data or handbook value.
		The data from this structure contribute to the range of values used to characterize this substance. There were no data on purity.
Test substance	:	Read across data for CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters. The data range represents diisooheptyl phthalate ester (CAS No. 71888-89-6) and 1,2-benzenedicarboxylic acid, dinonyl ester, branched and linear (CAS No. 68515-45-7).
Reliability	:	(2) valid with restrictions Although the original reference was not retrieved and reviewed for quality, this robust summary has a reliability rating of 2 because the data are from a peer reviewed database.
Flag	:	Critical study for SIDS endpoint
08.06.2006		(5)
Value	:	= 77 °C
Decomposition	:	no, at °C
Sublimation	:	no
Method	:	other: calculated
Year	:	
GLP	:	
Test substance	:	other TS: CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Method	:	The calculated value was determined using MPBPWIN version 1.41, a subroutine within the computer program EPI Suite™ version 3.12. Melting Point estimations performed by MPBPWIN are based on the average result of the calculation methods of K. Joback and Gold and Ogle. Joback's Method is described in Joback, K.G. 1982. A Unified Approach to Physical Property Estimation Using Multivariate Statistical Techniques. In The Properties of Gases and Liquids. Fourth Edition. 1987. R.C. Reid, J.M. Prausnitz and B.E. Poling, Eds. The Gold and Ogle Method simply uses the formula $T_m = 0.5839T_b$, where T_m is the melting point in Kelvin and T_b is the boiling point in Kelvin.
Remark	:	The SMILES notation used in the calculation was: <chem>O=C(c1cccc1C(=O)OCCCCC(C)C)OCCCCCCC</chem>
Test substance	:	1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters (CAS No. 68515-41-3)
Reliability	:	(3) invalid
08.06.2006		(7)

2.2 BOILING POINT

Value	:	424 °C at 1013 hPa
Decomposition	:	no

2. Physico-Chemical Data

Id 68515-41-3
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Method : other: Boiling point calculation by MPBPWIN ver. 1.41 using calculation method of Stein and Brown
Year :
GLP :
Test substance : other TS: CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
08.06.2006 (7)

2.3 DENSITY

2.3.1 GRANULOMETRY

2.4 VAPOUR PRESSURE

Value : .0000000924 hPa at 25 °C
Decomposition : no
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Method : Vapor pressure calculation by MPBPWIN ver. 1.41 using calculation method of Grain.
Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
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2.5 PARTITION COEFFICIENT

Partition coefficient : octanol-water
Log pow : 8.47 at 25 °C
pH value :
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Method : Partition coefficient by LOGKOWWIN ver. 1.67 using an atom/fragment

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Remark : calculation method of Meylan and Howard.
: EPI Suite™ is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Reliability : (2) valid with restrictions
: This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
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2.6.1 SOLUBILITY IN DIFFERENT MEDIA

Solubility in : Water
Value : .206 other: ug/L at 25 °C
pH value :
concentration : at °C
Temperature effects :
Examine different pol. :
pKa : at 25 °C
Description :
Stable :
Deg. product :
Method : other: calculated
Year :
GLP :
Test substance : other TS: CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Method : Water solubility calculated using WSKOWN ver 1.41 based on Kow correlation method of Meylan and Howard. Kow used in calculation was 6.46.
Remark : EPI Suite™ is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Reliability : (2) valid with restrictions
: This robust summary has a reliability rating of 2 because the data are calculated.
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2.6.2 SURFACE TENSION

2.7 FLASH POINT

2.8 AUTO FLAMMABILITY

2.9 FLAMMABILITY

2.10 EXPLOSIVE PROPERTIES

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2.11 OXIDIZING PROPERTIES

2.12 DISSOCIATION CONSTANT

2.13 VISCOSITY

2.14 ADDITIONAL REMARKS

3. Environmental Fate and Pathways

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3.1.1 PHOTODEGRADATION

Type : air
Light source : Sun light
Light spectrum : nm
Relative intensity : 1 based on intensity of sunlight
INDIRECT PHOTOLYSIS
Sensitizer : OH
Conc. of sensitizer : 1500000 molecule/cm³
Rate constant : .0000000002057 cm³/(molecule*sec)
Degradation : 50 % after 6.2 hour(s)
Deg. product : not measured
Method : other (calculated)
Year :
GLP :
Test substance :

Method : Photodegradation rate calculated by AOPWIN ver. 1.91 based on the methods of Atkinson.
Remark : 50% degradation after 6.24 hrs or 0.52 days based on a 12-hour day. The computer program AOPWIN (atmospheric oxidation program for Microsoft Windows) (EPI SuiteTM, 2000) calculates a chemical half-life for a 12-hour day (the 12-hour day half-life value normalizes degradation to a standard day light period during which hydroxyl radicals needed for degradation are generated), based on an OH- reaction rate constant and a defined OH- concentration.
EPI SuiteTM is used and advocated by the US EPA for chemical property estimation.
Test substance : CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
This robust summary has a reliability rating of 2 because the data are calculated.
Flag : Critical study for SIDS endpoint
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3.1.2 STABILITY IN WATER

Type : abiotic
t1/2 pH4 : at °C
t1/2 pH7 : 4.7 year at 25 °C
t1/2 pH9 : at °C
Deg. product : not measured
Method : other (calculated)
Year :
GLP :
Test substance : other TS: CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters

Method : Hydrolysis rate calculated by HYDROWIN ver. 1.67, a subroutine of the computer program EPI SuiteTM version 3.12., that is based on work for EPA by T. Mill et al.
Remark : EPI SuiteTM is used by the US EPA for estimating chemico-physical properties of substances.
Test substance : CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters
Reliability : (2) valid with restrictions

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The value was calculated based on chemical structure as modeled by EPI Suite™. This robust summary has a reliability rating of 2 because the data are calculated and not measured.
: Critical study for SIDS endpoint

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3.1.3 STABILITY IN SOIL

3.2.1 MONITORING DATA

3.2.2 FIELD STUDIES

3.3.1 TRANSPORT BETWEEN ENVIRONMENTAL COMPARTMENTS

3.3.2 DISTRIBUTION

Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level I
Year : 1997

Method : The EQC Level I is a steady state, equilibrium model that utilizes the input of basic chemical properties including molecular weight, vapor pressure, and water solubility to calculate distribution within a standardized regional environment.

Physicochemical input values for the model to represent di-C7-9 phthalate ester were:

MW = 390.57

Temperature = 25C

Water Solubility = 0.000206 mg/L

Vapor Pressure = 0.00000924 Pa

Pow = 8.47

Melting Point = -47C (taken as midpoint between range: -48 and -45)

Result

Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment, suspended sediment, biota).
: Soil = 97.7%
Air = 0.0%
Water = 0.0%
Sediment = 2.2%
Suspended sed. = 0.1%
Biota = 0.0%

Test substance : CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters

Reliability : (2) valid with restrictions
This robust summary has a reliability rating of 2 because the data are calculated and not measured.

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Media : air - biota - sediment(s) - soil - water
Method : Calculation according Mackay, Level III

3. Environmental Fate and Pathways

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Year :

Remark : Physicochemical input values for the model to represent di-C7-9 phthalate ester were:
MW = 390.57
Temperature = 25C
Water Solubility = 0.000206 mg/L
Vapor Pressure = 0.00000924 Pa
Pow = 8.47
Melting Point = -47C (taken as midpoint between range: -48 and -45)

Emissions rates used in the calculation:

Compartment	Rate (kg/hr)
Air	1000
Water	1000
Soil	1000

Half-lives used in the calculation:

Compartment	Half-life (hr)
Air	12.5a
Water	120b
Soil	420c
Sediment	420c

a - as calculated using AOPWIN version 1.91, a subroutine of the computer program EPI Suite™ version 3.12 and normalized to a 24 hour day [Environmental Protection Agency (EPA) (2000). EPI Suite™, Estimation Program Interface Suite, v3.12. U.S. EPA, Washington, DC, USA.]

b - based on biodegradation data from EBSI (1995) and Boethling (2000): Exxon Biomedical Sciences, Inc. (1995). Ready Biodegradability, Manometric Respirometry. Study No. 199894A. Unpublished report (contains data for diisooheptyl and diisononyl phthalates).

Boethling R (2000). HPVC-Screening Tool: Using Ready and Inherent Biodegradability Data to Derive Input Data for the EQC Model, Appendix 10 in Environment Canada, Environmental Categorization for Persistence Bioaccumulation and Inherent Toxicity of Substances on the Domestic Substance List Using QSARs, Results of an international workshop hosted by Chemicals Evaluation Division of Environment Canada, Nov. 11-12, 1999, in Philadelphia, PA, USA.

c - based on Boethling, R. recommendation that half-lives of 3 to 4 times longer than surface water should be used for soil and sediment.

Distribution data from the equilibrium model provide basic information on the potential partitioning behavior of chemicals between selected environmental compartments (i.e., air, water, soil, sediment).

Result : Using the Mackay Level I calculation, the following distribution is predicted for di-C7-9 phthalate ester:

Compartment	%Distribution
Air	1.0
Water	8.1
Soil	68.8
Sediment	22.1

Test substance : CAS No. 68515-41-3; 1,2-benzenedicarboxylic acid, di-C7-9-branched and linear alkyl esters

3. Environmental Fate and Pathways

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Reliability

: (2) valid with restrictions

This robust summary has a reliability rating of 2 because the data are calculated.

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3.4 MODE OF DEGRADATION IN ACTUAL USE

3.5 BIODEGRADATION

3.6 BOD5, COD OR BOD5/COD RATIO

3.7 BIOACCUMULATION

3.8 ADDITIONAL REMARKS

4.1 ACUTE/PROLONGED TOXICITY TO FISH

Type : static
Species : Oncorhynchus mykiss (Fish, fresh water)
Exposure period : 96 hour(s)
Unit : mg/l
LL0 : = 1000
LL50 : > 1000
Limit test :
Analytical monitoring : no
Method : other: EPA-600/3-75-009 Methods for Acute Toxicity tests with Fish, Macroinvertebrates and Amphibians, 1975
Year : 1975
GLP : no
Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-40-2)

Result : Nominal test concentrations:
 Loading Level (mg/L) Mortality (96h)
 Control 0
 100 0
 180 0
 320 0
 560 0
 1000 0

LL0 = 1000 mg/L
 LL50 > 1000 mg/L

No mortality was observed.
 No test substance insolubility was noted in report.

Test condition : Fish mean total length = 32.7 mm; fish mean wet weight = 0.47g; fish loading was not calculated.
 The test treatments were prepared by individually mixing the appropriate amount of test substance with 10ml of acetone and adding it directly to the test chambers. The control also received 10ml of solvent. One replicate was prepared for each test treatment and control. The test was performed in 5-gallon glass vessels containing 15L of dilution water. The dilution water was filter well water. Each treatment vessel contained 10 fish.

Test substance : Test temperature=12 +/- 1 Deg C., The pH range was 7.5 to 7.9. The Dissolved Oxygen ranged from 8.0 to 8.9mg/L. Fish were obtained from Fender's Fish Hatchery in Baltic, Ohio, USA.
 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS# 68515-40-2)
 No information on purity.
Conclusion : Test substance is non-toxic to fish at or below its water solubility level.
Reliability : (1) valid without restriction
 This summary is rated a "1" and represents a key study because it followed an U.S. EPA standard guideline, which describes a procedure specifically designed to evaluate this endpoint, and the results were reviewed for reliability and assessed as valid.

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4.2 ACUTE TOXICITY TO AQUATIC INVERTEBRATES

4. Ecotoxicity

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Type	:	static
Species	:	Daphnia magna (Crustacea)
Exposure period	:	48 hour(s)
Unit	:	mg/l
Analytical monitoring	:	no
Method	:	OECD Guide-line 202
Year	:	1997
GLP	:	yes
Test substance	:	other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)
Result	:	<p>LL50 > 1.0 mg/L, based on nominal loading level of the test substance.</p> <p>LC50 > 0.8 mg/L, based on analytical measurements for chronic study run subsequently with same material at same loading level.</p> <p>NOEL = 1.0 mg/L (with 10 mg/L dispersant), based on nominal loading level.</p> <p>No immobilization or flotation effects were observed over the 48-hour test period in either the 1 mg/L test treatment or controls.</p>
Test condition	:	<p>Test substance exposure solutions were prepared by adding 1 mg/L of the test substance and 10 mg/L of dispersant (Marlowet 40) to one liter of dilution medium. The dilution medium was Elendt's medium (Elendt and Bias, 1990), which was pH adjusted to 8 and aerated for >2 hours prior to use.</p> <p>Two replicate test systems, containing five daphnids each (< 24 hours old), were prepared for the single treatment, control and dispersant control. Test chambers were glass beakers with loose fitting lids. Each beaker contained 80 ml of exposure solution with a depth of approximately 5 cm. The study was conducted under static conditions in a temperature controlled room.</p> <p>Test temperature was 20 ± 1 Deg C., Lighting was 16 hours light : 8 hours dark with a 15 minute transition period. Other water quality parameters included: Water hardness = >140 mg/L (as CaCO₃), Alkalinity = >100 mg/L (as CaCO₃), pH = approximately 8, Dissolved oxygen = 8-9 mg/L.</p>
Test substance	:	Organisms were supplied by in-house continuous cultures. Age = <24 hours old. Test organisms were not fed during the study.
Conclusion	:	1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). No information on purity.
Reliability	:	<p>Test substance is not considered to be acutely toxic to aquatic organisms. Testing was conducted at a loading that exceeds the water solubility of the test substance after it was demonstrated that such a procedure was able to satisfactorily disperse the test substance and prevent flotation of the test organism (a documented problem that can occur when evaluating the toxicity of similar substances).</p> <p>(2) valid with restrictions</p> <p>The study was performed as a limit test. Analytical measurements of the test treatments were not performed during the acute test, however, analytical measurements of the test substance were performed during a subsequent chronic study at the same loading level and using the same treatment preparation. Test substance concentrations in the acute study are expected to be similar based on the chronic study analytical results.</p>
Flag	:	Critical study for SIDS endpoint
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4.3 TOXICITY TO AQUATIC PLANTS E.G. ALGAE

Species : Selenastrum capricornutum (Algae)
Endpoint :
Exposure period : 96 hour(s)
Unit : mg/l
Limit test :
Analytical monitoring : no
Method : other: EPA, Algal Assay Procedure: Bottle Test, 1971
Year : 1971
GLP : yes
Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-40-2)

Result : Nominal test concentrations: control, 56, 100, 180, 320, 560 and 1000 mg/L.

Loading Level (mg/L)	% Difference at 96h	
	Chlorophyll	Cell #
Control	---	---
56	-8	-6
100	-12	-6
180	-18	-19
320	-20	-24
560	-55	-63
1000	-61	-69

In-vivo chlorophyll, was measured daily. Both cell numbers and in-vivo chlorophyll, measured at termination.
Chlorophyll measured using a Turner filter fluorometer. Cell counts performed via a hemacytometer.

No final cell counts reported.

Limited details on test treatment preparation in report.

"Globules" of test material were observed in all test flasks during the study.

Test condition : The appropriate amount of test substance was added directly to algal growth medium (control and diluent) to form individual treatment concentrations. The test was performed in 125 ml flasks. The initial algal concentration was 3.0 E4 cells/ml.

Lighting = 4,000 lux, Test temperature = 24+/-1 Deg C. The pH range was 7.2 to 7.6. Algal culture stock obtained from U.S. EPA Environmental Research Laboratory, Corvallis, Oregon.

Test substance : 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS# 68515-40-2)

No information on purity.

1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS# 68515-40-2)

No information on purity.

Conclusion : A EC50 cannot be calculated because the test is not valid due to excess undissolved test material.

Reliability : (3) invalid

The observed toxicity was due to physical effects. The test substance coated the organisms.

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4.4 TOXICITY TO MICROORGANISMS E.G. BACTERIA

4.5.1 CHRONIC TOXICITY TO FISH

4.5.2 CHRONIC TOXICITY TO AQUATIC INVERTEBRATES

Species : Daphnia magna (Crustacea)
Endpoint : reproduction rate
Exposure period : 21 day(s)
Unit : mg/l
NOEC : = .82
LC50 : > .82
Analytical monitoring : yes
Method : OECD Guide-line 202, part 2 "Daphnia sp., Reproduction Test"
Year : 1984
GLP : yes
Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)

Method : The test method followed the Daphnid chronic testing procedure described in OECD guideline 202 (1984) with the use of a dispersant, castor oil 40-ethoxylate (Marlowet 40), in accordance with guideline specifications.

Result : Daphnia parent (Po) survival, reproduction (cumulative number of offspring, F1, per live parent), and parent length were evaluated as the biological endpoints. Di-heptyl/nonyl phthalate ester showed no effect on survival, reproduction, and length at a loading of 1.0 mg/L test substance and 10 mg/L dispersant under the conditions of this test.

	Control	Dispersant	Control	Test Substance
Po % Mortality	0	20		10
Mean F1/				
Surviving Po	120 (sd=13.3)	131 (sd=23.5)		151 (sd=8.8)
Po Mean Length	4.2 (sd=0.14)	4.3 (sd=0.16)		4.2 (sd=0.16)

Test condition : Test substance exposure solutions were prepared using stock dispersions prepared by adding 100 mg substance and 1000 mg dispersant (castor oil 40-ethoxylate; Marlowet 40), then bringing the test solution to 1 L by adding dilution medium. The dilution medium was Elendt's medium (Elendt and Bias, 1990), which was pH adjusted to 8 and aerated for >2 hours prior to use.

Ten replicate test systems with 1 daphnid each (< 24 hours old) were prepared in glass beakers with loose fitting lids. Each beaker contained 80 ml of exposure solution with a depth of approximately 5 cm. The photoperiod was controlled to 16 hours light and 8 hours dark with a 15 minute transition period.

The exposure solution was renewed every Monday, Wednesday, and Friday. On each renewal day the parent organism (Po) was transferred to a new exposure solution and neonates (F1) were counted. Water quality measurements including dissolved oxygen concentration and pH were determined at every renewal for the new and old exposure and control solutions. Test conditions were:

Temperature = 20 +/- 1.0 degree C
 Water hardness = >140 mg/L (as CaCO3)
 Alkalinity = >100 mg/L (as CaCO3)
 pH = approximately 8
 Dissolved oxygen = 8-9 mg/L

Standard daily feeding rates with the cultured alga, *Chlorella vulgaris*, was supplemented with microencapsulated food, "Frippak Booster".

	<p>Test substance analyses of new and old exposure solutions were performed using gas chromatography with flame ionization detection, after a hexane extraction. The mean measured test substance concentrations for the 21-day period were 0.93 mg/L in new exposure solutions and 0.72 mg/L in old exposure solutions, which represents 92 and 72%, respectively, of the nominally added test substance.</p>
Test substance	: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3); purity >99.5%
Conclusion	: Invertebrate (<i>Daphnia magna</i>) toxicity data reported for di-heptyl/nonyl phthalate ester are consistent with valid data for several high molecular weight phthalate esters as summarized by Brown et al. (1998) (these data), Staples et al. (1997), and Rhodes et al. (1995). These data show that high molecular weight phthalate esters, including di-heptyl/nonyl phthalate ester, do not produce acute toxicity to <i>Daphnia magna</i> . Testing was conducted at a loading that exceeds the water solubility of diisoheptyl and diisononyl phthalate esters (0.017 mg/L and 0.61 ug/L; Letinski et al., 2002) after it was demonstrated that such a procedure was able to satisfactorily disperse the test substance and that it prevented floatation of the test organism, a documented problem that can occur when evaluating the toxicity of similar substances.
Reliability	: (1) valid without restriction The study procedure followed an accepted test guideline and applied GLP. The study procedure and results were accepted in a peer-reviewed journal. The data are consistent with known toxicological properties of similar high molecular weight phthalate ester substances.
Flag 07.12.2006	: Critical study for SIDS endpoint

(3)

4.6.1 TOXICITY TO SEDIMENT DWELLING ORGANISMS**4.6.2 TOXICITY TO TERRESTRIAL PLANTS****4.6.3 TOXICITY TO SOIL DWELLING ORGANISMS****4.6.4 TOX. TO OTHER NON MAMM. TERR. SPECIES****4.7 BIOLOGICAL EFFECTS MONITORING****4.8 BIOTRANSFORMATION AND KINETICS****4.9 ADDITIONAL REMARKS**

5.0 TOXICOKINETICS, METABOLISM AND DISTRIBUTION

5.1.1 ACUTE ORAL TOXICITY

Type : LD50
Value : > 19300 mg/kg bw
Species : rat
Strain : other: Carworth Farm E (CFE)
Sex : male/female
Number of animals : 8
Vehicle : other: none
Doses : single
Method : other
Year :
GLP : no data
Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)

Remark : Four rats of each sex at each dose level (unspecified number of doses).
 Hair appeared persistently wet at unspecified dose levels in treated animals.

Source : BP Chemicals Ltd. London
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). Approximately 45% C7, 40% C8 and 15% C9 w/w; at least 80% linear; purity unspecified.

Reliability : (2) valid with restrictions
 Pre-GLP study from peer reviewed literature.

Flag : Critical study for SIDS endpoint
 07.12.2006 (4)

Type : LD50
Value : > 20000 mg/kg bw
Species : rat
Strain : other: CFE
Sex : male/female
Number of animals : 10
Vehicle : other: none
Doses : single
Method : other
Year :
GLP : no data
Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)

Remark : Single doses were administered by gavage to groups of five rats of each sex, and animals observed for 14 days.
 The only overt effects seen were slight diarrhoea and matting of the fur with an oily substance resembling the test material. Autopsy revealed no effects (the extent of examination was not specified).

Source : BP Chemicals Ltd. London
 EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). The test material consisted of esters of phthalic acid and mixed alcohols with 7-9 carbon atoms (Alphanol 79); purity unspecified.

5. Toxicity

Id 68515-41-3

Date 07.12.2006

Reliability	: Di-heptyl/nonyl Phthalate Ester (CAS No. 68515-41-3)	
Flag	: (2) valid with restrictions	
07.12.2006	: Pre-GLP study from peer reviewed literature.	
	: Critical study for SIDS endpoint	(9)
Type	: LD50	
Value	: > 19300 mg/kg bw	
Species	: mouse	
Strain	: other: Carworth Farm (CF1)	
Sex	: male/female	
Number of animals	: 8	
Vehicle	: other: none	
Doses	: single	
Method	: other	
Year	:	
GLP	: no data	
Test substance	: other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)	
Remark	: Four mice of each sex at each dose level (unspecified number of doses). Wet hair was observed in the perianal area at unspecified dose levels.	
Source	: BP Chemicals Ltd. London EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	
Test substance	: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). Approximately 45% C7, 40% C8 and 15% C9 w/w; at least 80% linear; purity unspecified.	
Reliability	: (2) valid with restrictions	
Flag	: Pre-GLP study from peer reviewed literature.	
07.12.2006	: Critical study for SIDS endpoint	(4)
Type	: LD50	
Value	: > 20000 mg/kg bw	
Species	: mouse	
Strain	: other: CFW	
Sex	: male/female	
Number of animals	: 20	
Vehicle	: other: none	
Doses	: single	
Method	: other	
Year	:	
GLP	: no data	
Test substance	: other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)	
Remark	: Single doses were administered by gavage to groups of ten mice of each sex, and animals observed for 14 days. The only overt effects seen were slight diarrhoea and matting of the fur with an oily substance resembling the test material. Autopsy revealed no effects (the extent of examination was not specified).	
Source	: BP Chemicals Ltd. London EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)	
Test substance	: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). The test material consisted of esters of phthalic acid and mixed alcohols with 7-9 carbon atoms (Alphanol 79); purity unspecified.	
Reliability	: (2) valid with restrictions	
Flag	: Pre-GLP study from peer reviewed literature.	
	: Critical study for SIDS endpoint	

07.12.2006

(9)

5.1.2 ACUTE INHALATION TOXICITY**5.1.3 ACUTE DERMAL TOXICITY****5.1.4 ACUTE TOXICITY, OTHER ROUTES****5.2.1 SKIN IRRITATION**

Species : rabbit
Concentration : undiluted
Exposure : Occlusive
Exposure time : 6 hour(s)
Number of animals : 8
Vehicle : other: none
PDII :
Result : not irritating
Classification : not irritating
Method : other
Year :
GLP : no data
Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)

Remark : Covered application of 1 ml neat material to the shaven back of New Zealand white rabbits (probably two in number but possibly four of each sex) for 6 hr/day, daily for 3 days. Skin assessed visually and using intravenous sulpham blue, probably daily, for up to 7 days. At 7 days, the skin was also examined histologically.

Source : BP Chemicals Ltd. London
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). Approximately 45% C7, 40% C8 and 15% C9 w/w; at least 80% linear; purity unspecified.

Reliability : (2) valid with restrictions
Pre-GLP study from peer reviewed literature.

Flag : Critical study for SIDS endpoint

07.12.2006

(4)

5.2.2 EYE IRRITATION

Species : rabbit
Concentration : undiluted
Dose : .1 ml
Exposure time : unspecified
Comment : no data
Number of animals :
Vehicle : no data
Result : not irritating
Classification : not irritating
Method : other
Year : 1964

5. Toxicity

Id 68515-41-3

Date 07.12.2006

GLP : no data
Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)
Remark : Method was that described in the US Federal Register 29 FR 13009, 1964. Irritancy assessment was based on the recommendations of the US DHEW, 1964.
Source : BP Chemicals Ltd. London
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). Approximately 45% C7, 40% C8 and 15% C9 w/w; at least 80% linear; purity unspecified.
Reliability : (2) valid with restrictions
Pre-GLP study from peer reviewed literature.
Flag : Critical study for SIDS endpoint
07.12.2006 (4)

5.3 SENSITIZATION

Type : other
Species : guinea pig
Number of animals : 10
Vehicle :
Result : not sensitizing
Classification : not sensitizing
Method : other
Year :
GLP : no data
Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)
Remark : Induction period: Undisclosed amounts of 0.1% w/v solutions in light liquid paraffin were injected subcutaneously, or applied dermally (apparently uncovered), to the shaven back of five male and five female guinea-pigs on 3 days a week.

Challenge: After a 10-day period without treatment, the animals were given a challenge to consisting of a dermal (apparently uncovered) application to the right flank. Animals were examined visually at 1, 24 and 48 hours after challenge.

The whole induction and challenge procedures were then repeated on the same animals.
Source : BP Chemicals Ltd. London
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)
Test substance : 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). Approximately 45% C7, 40% C8 and 15% C9 w/w; at least 80% linear; purity unspecified.
Reliability : (2) valid with restrictions
Pre-GLP study from peer reviewed literature.
Flag : Critical study for SIDS endpoint
07.12.2006 (4)

5.4 REPEATED DOSE TOXICITY

Type : Sub-chronic
Species : rat

5. Toxicity

Id 68515-41-3

Date 07.12.2006

Sex : male/female
Strain : other: CFE
Route of admin. : oral feed
Exposure period : 90 days
Frequency of treatm. : continuous
Post exposure period : none
Doses : 0, 0.125, 0.25, 0.5, 1.0 % (60, 120, 240 and 480 mg/kg/day); groups of 15 animals/sex/dose
Control group : yes, concurrent no treatment
NOAEL : = .125 %
LOAEL : = .25 %
Method : other
Year :
GLP : no data
Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)

Remark : Animals were Carworth Farm E (CFE) strain. All animals were subjected to gross and histopathological examination of a wide range of organs and tissues, as well as urinalysis, haematology and serum chemistry examination. The findings suggested a slight anaemia at dietary levels of 0.25% and above and indicated an effect on the liver and kidney, particularly at 0.5 and 1.0%.

Result : At 0.125% [approximately 60 mg/kg bw/day] there were no overt effects or changes in haematology, serum chemistry, urinalysis or in a gross and microscopic examination of a wide range of tissues. At 0.25% and above there were indications of decreased haemoglobin levels and red blood cell counts, as well as increased urinary cell excretion. At 0.5% and above haematocrit, haemoglobin and red blood cell counts were clearly reduced, while relative liver and kidney weights were increased. At 1.0% males grew more slowly and were unable to concentrate urine normally, while two males produced renal casts. Relative weights of the brain and gonads were increased in males, and both sexes had increased haemosiderin in the spleen.

Source : BP Chemicals Ltd. London

Test substance : EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). The test material consisted of the esters of phthalic acid and mixed alcohols with 7-9 carbon atoms (Alphanol 79); purity unspecified.

Reliability : (2) valid with restrictions
Pre-GLP study from peer reviewed literature.

Flag : Critical study for SIDS endpoint

07.12.2006

(9)

Type : Sub-chronic
Species : rabbit
Sex : male/female
Strain : New Zealand white
Route of admin. : dermal
Exposure period : 3 weeks
Frequency of treatm. : daily, 5 days/week
Post exposure period : none
Doses : 1 ml neat material; 1 animal/sex
Control group : no
NOAEL : = 100 %
Method : other
Year :
GLP : no data

5. Toxicity

Id 68515-41-3

Date 07.12.2006

Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)

Remark : Uncovered application of 1 ml neat material to the shaven back of rabbits. The skin was assessed visually on a daily basis and by histological examination on the day after the final application.

Result : NOEL = neat material. No irritation was seen.

Source : BP Chemicals Ltd. London
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). Approximately 45% C7, 40% C8 and 15% C9 w/w; at least 80% linear; purity unspecified.

Reliability : (2) valid with restrictions
Pre-GLP study from peer reviewed literature.

Flag : Critical study for SIDS endpoint
07.12.2006 (4)

Type : Sub-chronic

Species : guinea pig

Sex : male/female

Strain : no data

Route of admin. : dermal

Exposure period : 3 weeks

Frequency of treatm. : daily, 5 days/week

Post exposure period : none

Doses : 0.5 ml neat material; 5 animals/sex

Control group : no

NOAEL : = 100 %

Method : other

Year :

GLP : no data

Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)

Remark : Uncovered application of 0.5 ml neat material to the shaven back of five albino guinea-pigs (both sexes were tested.)
Skin was assessed visually on a daily basis and by histological examination on the day after the final application.

Result : LOEL = neat material. The skin became coarse, slightly thickened and some sloughing of the surface layers was apparent.

Source : BP Chemicals Ltd. London
EUROPEAN COMMISSION - European Chemicals Bureau Ispra (VA)

Test substance : 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). Approximately 45% C7, 40% C8 and 15% C9 w/w; at least 80% linear; purity unspecified.

Reliability : (2) valid with restrictions
Pre-GLP study from peer reviewed literature.

Flag : Critical study for SIDS endpoint
07.12.2006 (4)

Type :

Species : rat

Sex : male/female

Strain : other: not specified

Route of admin. : oral feed

Exposure period : 4 weeks

Frequency of treatm. : daily

Post exposure period :

Doses : not stated

5. Toxicity

Id 68515-41-3

Date 07.12.2006

Control group : yes
NOAEL : = 100 mg/kg
Method : other: not specified
Year : 1973
GLP : no data
Test substance : other TS: unspecified DIOP

08.06.2006

(12)

5.5 GENETIC TOXICITY 'IN VITRO'

Type : Mouse lymphoma assay
System of testing : Mammalian Cell
Test concentration : 0.125 to 6 ul/ml
Cycotoxic concentr. :
Metabolic activation : with and without
Result : negative
Method : OECD Guide-line 476
Year : 2000
GLP : yes
Test substance : other TS: Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515

Method : Control Groups:
The negative control article was the solvent (acetone) used in the assay. Ethylmethane sulfonate (EMS) was used as a positive control in the assays without S9 activation. 3-methylcholanthrene which requires metabolic activation, was used as a positive control for assays with S9.

Statistical Methods:

The minimum criterion necessary to demonstrate mutagenesis was a mutation frequency that was at least 1.5 times the concurrent background frequency plus 10×10^{-6} . The background frequency was defined as the average mutant frequency of the solvent negative controls.

Result : In the absence of activation, 0.75 to 6.0 ul/ml induced moderate to high toxicity (percent relative growths: 3.2% to 48.4%), but only a slight increase in mutation frequency at the highest doses. In the presence of a metabolic fraction, 0.125 to 1.5 ul/ml resulted in percent relative growths of 8.9% to 82.2% without increasing the incidence of mutations. Thus, the test compound was considered non-mutagenic in this assay.

Test condition : Mouse lymphoma cells were seeded into a series of tubes at 6×10^6 cells per tube. Dosed tubes were exposed for 4 hours to the test substance. An expression period of 48 hours was used; after the 48 hour expression time, 3×10^6 cells per plate were added to semi-solid selection medium containing 3 ug/ml trifluorothymidine (TFT) to score for mutant colonies and 200 cells per plate were added to cloning medium, without TFT, to evaluate viability. Mutant frequencies were calculated after 10-14 days incubation. Mutant and total colony count at each dose level were determined by triplicate plates.

Test substance : Commercial test substance, 711P, is actually an equal composition mixture of six phthalate esters consisting of C7, C9, and C11 ester side chains. This test substance is considered by EPA under the following CAS nos.: 68515-44-6 (di C7), 68515-45-7 (di C9), 3648-20-2 (di C11), 111381-89-6 (C7, C9), 111381-90-9 (C7, C11), and 111381-91-0 (C9, C11).

Conclusion : Under conditions of this study the test substance was non-mutagenic in the mouse lymphoma assay with or without metabolic activation.

Reliability : (1) valid without restriction
07.12.2006

(2)

5.6 GENETIC TOXICITY 'IN VIVO'

5.7 CARCINOGENICITY

5.8.1 TOXICITY TO FERTILITY

Type	: Two generation study
Species	: rat
Sex	: male/female
Strain	: Sprague-Dawley
Route of admin.	: oral feed
Exposure period	: Continuous throughout study
Frequency of treatm.	: Daily over two generations
Premating exposure period	
Male	: 10 weeks
Female	: 10 weeks
Duration of test	: 2 generation
No. of generation studies	:
Doses	: 0.0, 0.1, 0.5, or 1.0%.
Control group	: yes
NOAEL parental	: = 1 %
NOAEL F1 offspring	: = 1 %
other: systemic effects	: = .5 %
Method	: EPA OPPTS 870.3800
Year	: 2000
GLP	: yes
Test substance	: other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)
Method	: Statistical Methods: Organ and body weight data assessed by Bartlett's test for homogeneity of variance; then pairwise comparisons by Behren's-Fisher test or Dunnett's test. Intergroup differences in macroscopic and microscopic pathology assessed by Fisher's exact test. Food consumption and litter data analyzed by ANOVA (parametric) or Kruskal-Wallis test (non-parametric) as appropriate.
Remark	: The 1.0% males showed reduced body weights in both the F0 and F1 generations. There was no impairment of fertility, fecundity, or development in either generation, but pup body weights were slightly reduced in the 1.0% group over the weaning period. Ovary weights were decreased in the 1.0% group for both generations, although ovarian function as assessed by estrus cycle and mating behavior was not affected. Liver changes indicative of peroxisomal proliferation were noted in both generations and both sexes at the high dose (1%), characterized by increased liver weight in young rats, histopathological changes and decreased weights in mature rats, and an increase in palmitoyl CoA oxidase activity.
Result	: NOAEL - 1.0% in diet for reproductive endpoints; 0.5% for general toxicity.
Test condition	: F0 males and females (28 animals/sex) were exposed to the test substance for 10 weeks prior to mating. One male and one female were paired for up to 3 weeks. F0 offspring were examined 24 hours after birth and number of pups, body weights, sex, and gross observations. Litters were culled to 4 male and 4 female pups and at PND 25 selected for the next (F1) generation. Parental (F0) males and females were necropsied, organs weighed and microscopically examined. Epididymal fluid was obtained for sperm analysis, uteri were examined for implantation sites.

5. Toxicity

Id 68515-41-3

Date 07.12.2006

Livers from five males/group were analyzed for protein content and cyanide-insensitive palmitoyl CoA oxidase activity. Body weights and food consumption were recorded weekly throughout the study, and clinical observations recorded twice daily

Test substance : 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). Bisoflex L79P (di-(C7-C9 alkyl), is a phthalate ester based upon a linear alcohol, Linevol 79. Linevol 79 has alkyl chains with carbon distributions of >96% in the range C7 to C9 (typically 39 to 50% C7, 17 to 28% C8, and 27 to 39% C9). Linevol 79 has a minimum of 80% normality with predominant mono-2-methyl branching.

Conclusion : The test substance did not impair reproductive function in rats at any level tested. Signs of systemic toxicity were observed at 1.0%.

Reliability : (1) valid without restriction

Flag : Critical study for SIDS endpoint

07.12.2006 (13)

5.8.2 DEVELOPMENTAL TOXICITY/TERATOGENICITY

Species : rat

Sex : male/female

Strain : Sprague-Dawley

Route of admin. : gavage

Exposure period : GD 1 through GD 19

Frequency of treatm. : daily

Duration of test : 20 days

Doses : 250, 500, or 1000 mg/kg/day

Control group : yes, concurrent vehicle

NOAEL maternal tox. : = 1000 mg/kg bw

NOAEL teratogen. : = 500 - mg/kg bw

Result : NOAEL for maternal toxicity = 1000 mg/kg/day; NOAEL for developmental toxicity = 500 mg/kg/day, based on minor skeletal and visceral variations. No malformations were observed at any dose level.

Method : EPA OPPTS 870.3700

Year : 2001

GLP : yes

Test substance : other TS: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3)

Method : For statistical analysis: Homogeneity of variance was assessed using Bartlett's test, and data were analyzed with parametric tests (analysis of variance followed by Williams' test) or nonparametric tests (Kruskal-Wallis followed by Shirley's test) as appropriate. Data on fetal malformations and variations was analyzed using categorical data models.

Remark : There were no effects on the incidence of external or visceral abnormalities. An increased incidence of dilated renal pelvis was observed in the group treated with 250 mg/kg/day, but there was not a significant trend with treatment. Three fetuses from 2 litters in the 1000 mg/kg/day group exhibited premature termination of the vertebral column, and another fetus from a third litter had a shortened tail. These types of findings occur quite frequently and are considered unrelated to treatment. An increased incidence of supernumerary lumbar ribs was observed in the high (1000 mg/kg/day) dose group. However, these minor variations are commonly observed in rodents and are not considered to be an indicator of a teratogenic effect. There were no statistically significant differences in bodyweight, fertility, reproductive organs, litter size, placental weights or fetal survival between any treatment groups and the prospective control groups at any time during gestation. There were no remarkable macroscopic findings in the maternal animals at necropsy. Fetal, litter, and placental weights were all unaffected by treatment. Under the conditions of this study, the test substance did not induce any evidence of maternal

	toxicity, embryofetal lethality or teratogenicity. The NOAEL for maternal toxicity was 1000 mg/kg/day and the developmental NOAEL was 500 mg/kg/day, based on minor skeletal and visceral variations. No malformations were observed at any dose level.
Test condition	: A total of 220 virgin female Sprague-Dawley rats were mated on a 1:1 basis with stock males from the same strain and source. The day that a positive indication of mating was observed (i.e., sperm-positive vaginal smear or at least three copulation plugs) was designated Day 0 of gestation (GD0). Females showing a positive indication of mating were allocated to treatment groups. Each group consisted of 22 timed pregnant females (approximately 10-11 weeks of age, weighing 210-267 grams). Animals were dosed by gavage once daily from GD1-19 at doses of 250, 500, or 1000 mg/kg/day; vehicle controls received olive oil. Animals were observed twice daily; bodyweight was measured daily as was food consumption. Dams were euthanized with CO2 on GD20 and were weighed and examined macroscopically for signs of disease or adverse reactions to treatment. The reproductive tract, including ovaries, were removed and assessed for gravid uterine weight, number of corpora lutea in each ovary, numbers of implantation and resorption sites, and number and distribution of fetuses in each uterine horn. Fetuses were identified with respect to their position in the uterine horn. Each fetus was weighed, sexed, examined for external abnormalities, and euthanized. Each placenta was weighed and examined. Approximately half of each litter was allocated to skeletal examination and were given a visceral examination prior to evisceration and fixation in methylated spirit. Staining was done with Alizarin Red, using a modification of the Dawson staining technique. The remainder of the fetuses were fixed in Bouin's Fluid prior to examination by the Wilson free-hand serial sectioning technique.
Test substance	: 1,2-benzenedicarboxylic acid, di-C7-9 branched and linear alkyl ester (CAS No. 68515-41-3). Bisoflex L79P: di-C7-C9 alkyl phthalate CAS 68515-41-3 is a phthalate ester based on predominantly linear alcohol, Linevol 79; alkyl chain with a carbon distribution of greater or equal to 96% in the range C7-C9 (typically 39-50% C7, 17-28% C8 and 27-39% C9); with minimum 80% normality and predominantly mono-2-methyl branching.
Conclusion	: Under the conditions of the study, the test substance did not induce any evidence of maternal toxicity, embryofetal lethality or teratogenicity.
Reliability	: (1) valid without restriction
Flag	: Critical study for SIDS endpoint
07.12.2006	

(8)

5.8.3 TOXICITY TO REPRODUCTION, OTHER STUDIES

5.9 SPECIFIC INVESTIGATIONS

5.10 EXPOSURE EXPERIENCE

5.11 ADDITIONAL REMARKS

6.1 ANALYTICAL METHODS

6.2 DETECTION AND IDENTIFICATION

7.1 FUNCTION

7.2 EFFECTS ON ORGANISMS TO BE CONTROLLED

7.3 ORGANISMS TO BE PROTECTED

7.4 USER

7.5 RESISTANCE

8.1 METHODS HANDLING AND STORING

8.2 FIRE GUIDANCE

8.3 EMERGENCY MEASURES

8.4 POSSIB. OF RENDERING SUBST. HARMLESS

8.5 WASTE MANAGEMENT

8.6 SIDE-EFFECTS DETECTION

8.7 SUBSTANCE REGISTERED AS DANGEROUS FOR GROUND WATER

8.8 REACTIVITY TOWARDS CONTAINER MATERIAL

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10. Summary and Evaluation

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10.1 END POINT SUMMARY

10.2 HAZARD SUMMARY

10.3 RISK ASSESSMENT